



# wwPDB X-ray Structure Validation Summary Report

Jun 23, 2014 – 05:35 PM EDT

PDB ID : 4N4V  
Title : Co-crystal structure of tankyrase 1 with compound 4 [(4S)-3-{trans-4-[6-amino-5-(pyrimidin-2-yl)pyridin-3-yl]cyclohexyl}-5,5-dimethyl-4-phenyl-1,3-oxazolidin-2-one]  
Authors : Huang, X.  
Deposited on : 2013-10-08  
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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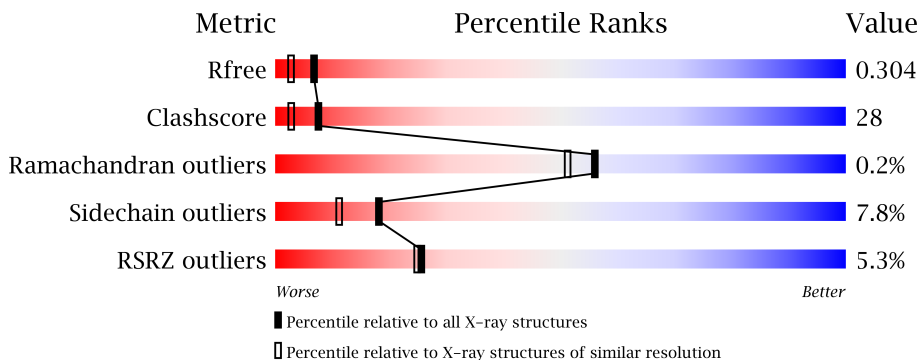
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	2GY	A	1402	-	X
3	2GY	B	1402	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3734 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

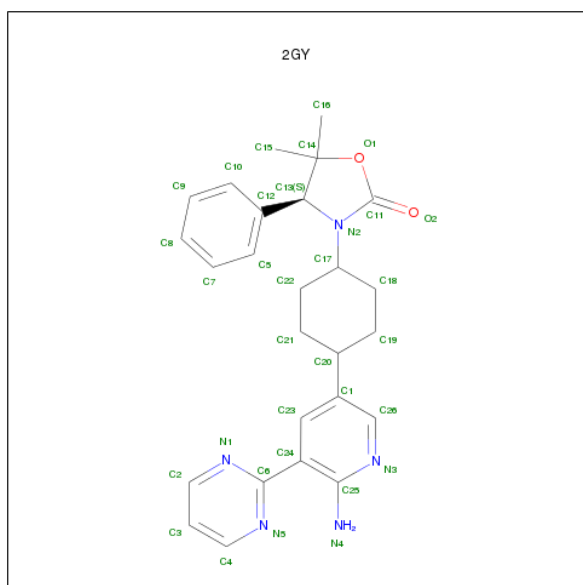
- Molecule 1 is a protein called Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1697	1068	310	307	12			
1	B	202	Total	C	N	O	S	0	0	0
			1615	1016	294	294	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (4S)-3-{TRANS-4-[6-AMINO-5-(PYRIMIDIN-2-YL)PYRIDIN-3-YL]CYCLOHEXYL}-5,5-DIMETHYL-4-PHENYL-1,3-OXAZOLIDIN-2-ONE (three-letter code: 2GY) (formula: C<sub>26</sub>H<sub>29</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 33	C 26	N 5	O 2	0	0
3	B	1	Total 33	C 26	N 5	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total 201	O 201	0	0
4	B	153	Total 153	O 153	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.99Å 77.72Å 147.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 41.61 – 1.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 93.4 (41.61-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.97Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.264 , 0.290 0.279 , 0.304	Depositor DCC
$R_{free}$ test set	1666 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	5 of 32865 reflections (0.015%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2GY, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	1/1740 (0.1%)	0.89	8/2339 (0.3%)
1	B	0.70	4/1655 (0.2%)	1.26	18/2225 (0.8%)
All	All	0.64	5/3395 (0.1%)	1.08	26/4564 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1266	MET	C-N	8.65	1.53	1.34
1	B	1122	GLU	CB-CG	7.03	1.65	1.52
1	B	1179	GLU	CB-CG	-6.21	1.40	1.52
1	B	1131	GLU	CB-CG	5.14	1.61	1.52
1	A	1130	ARG	CG-CD	5.09	1.64	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1133	ARG	NE-CZ-NH1	-26.86	106.87	120.30
1	B	1133	ARG	NE-CZ-NH2	18.87	129.74	120.30
1	B	1159	ARG	NE-CZ-NH1	-15.21	112.69	120.30
1	A	1130	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	B	1159	ARG	NE-CZ-NH2	10.82	125.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1159	ARG	Sidechain
1	B	1266	MET	Mainchain

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1630	83	0
1	B	1615	0	1532	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	28	2	0
3	B	33	0	29	4	0
4	A	201	0	0	27	2
4	B	153	0	0	37	2
All	All	3734	0	3219	182	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 182 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1190:ASN:HB2	4:B:1613:HOH:O	1.25	1.28
1:B:1175:ASN:HB3	4:B:1543:HOH:O	1.40	1.20
1:B:1263:PHE:HB2	4:B:1577:HOH:O	1.38	1.19
1:B:1176:HIS:HD2	4:B:1633:HOH:O	1.26	1.19
1:B:1314:GLU:HB2	4:B:1599:HOH:O	1.49	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1516:HOH:O	4:B:1508:HOH:O[4_455]	2.10	0.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1579:HOH:O	4:B:1607:HOH:O[4_455]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/217 (96%)	203 (97%)	6 (3%)	0	100	100
1	B	198/217 (91%)	190 (96%)	7 (4%)	1 (0%)	38	29
All	All	407/434 (94%)	393 (97%)	13 (3%)	1 (0%)	56	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1266	MET

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/185 (96%)	167 (94%)	11 (6%)	26	18
1	B	168/185 (91%)	152 (90%)	16 (10%)	12	7
All	All	346/370 (94%)	319 (92%)	27 (8%)	18	11

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1118	TYR
1	B	1133	ARG
1	B	1262	GLN

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Mol	Chain	Res	Type
1	B	1122	GLU
1	A	1178	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1217	ASN
1	A	1248	GLN
1	B	1177	HIS
1	A	1201	HIS
1	B	1174	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	211/217 (97%)	0.54	7 (3%) 44 44	18, 25, 34, 42	0
1	B	202/217 (93%)	0.74	15 (7%) 14 14	20, 28, 36, 43	0
All	All	413/434 (95%)	0.64	22 (5%) 25 25	18, 26, 36, 43	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1104	GLN	7.5
1	A	1104	GLN	7.5
1	B	1265	THR	6.7
1	B	1263	PHE	6.2
1	A	1284	VAL	3.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	2GY	A	1402	33/33	0.27	3.04	29,42,59,63	0
3	2GY	B	1402	33/33	0.24	2.33	35,47,64,68	0
2	ZN	A	1401	1/1	0.08	-2.44	26,26,26,26	0
2	ZN	B	1401	1/1	0.07	-2.93	29,29,29,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.